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OMB No. 0704-0188

1. REPORT DATE (DD-MM-YYYY)

3. DATES COVERED (From - To)

5a. CONTRACT NUMBER	
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5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER	
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5d. PROJECT NUMBER

2303

5e. TASK NUMBER	
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m268

5f. WORK UNIT NUMBER

345 709

8. PERFORMING ORGANIZATION REPORT

10. SPONSOR/MONITOR'S ACRONYM(S)	
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11. SPONSOR/MONITOR'S NUMBER(S)	
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Please see attached

Approved for public release; distribution unlimited.

13. SUPPLEMENTARY NOTES

14. ABSTRACT

20030129 233

16. SECURITY CLASSIFICATION OF:

17. LIMITATION OF ABSTRACT

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19a. NAME OF RESPONSIBLE PERSON

Leilani Richardson

a. REPORT

b. ABSTRACT

c. THIS PAGE

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19b. TELEPHONE NUMBER

(include area code)
(661) 275-5015

2303 Mar 2002

MEMORANDUM FOR PRS (In-House Publication)

FROM: PROI (STINFO)

22 March 2002

SUBJECT: Authorization for Release of Technical Information, Control Number: **AFRL-PR-ED-VG-2002-068**
Jeff Sheehy, et al. (PRSP), "Computational Chemistry Studies of HEDM"

AF Chief Scientists
(Edwards AFB, CA, 07 March 2002) (Deadline: Past Due)

(Statement A)

1. This request has been reviewed by the Foreign Disclosure Office for: a.) appropriateness of distribution statement, b.) military/national critical technology, c.) export controls or distribution restrictions, d.) appropriateness for release to a foreign nation, and e.) technical sensitivity and/or economic sensitivity.
Comments: _____

Signature _____ Date _____

2. This request has been reviewed by the Public Affairs Office for: a.) appropriateness for public release and/or b) possible higher headquarters review.
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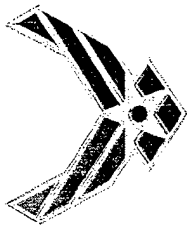
3. This request has been reviewed by the STINFO for: a.) changes if approved as amended, b) appropriateness of references, if applicable; and c.) format and completion of meeting clearance form if required
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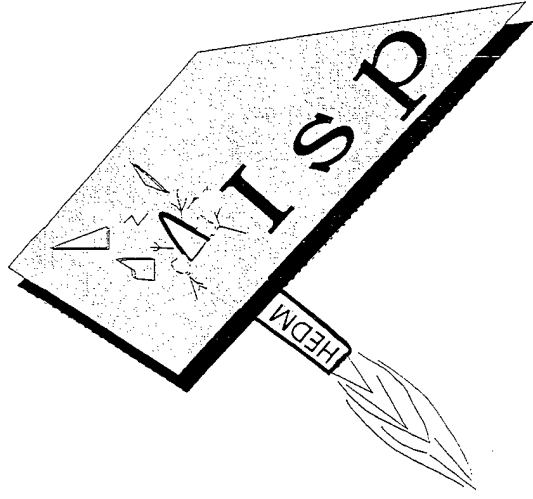
4. This request has been reviewed by PR for: a.) technical accuracy, b.) appropriateness for audience, c.) appropriateness of distribution statement, d.) technical sensitivity and economic sensitivity, e.) military/national critical technology, and f.) data rights and patentability
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APPROVED/APPROVED AS AMENDED/DISAPPROVED

PHILIP A. KESSEL Date
Technical Advisor
Space and Missile Propulsion Division



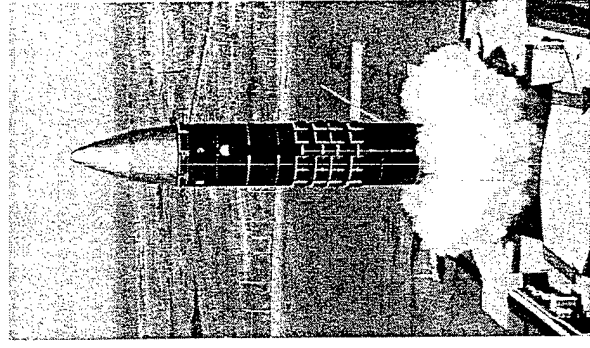
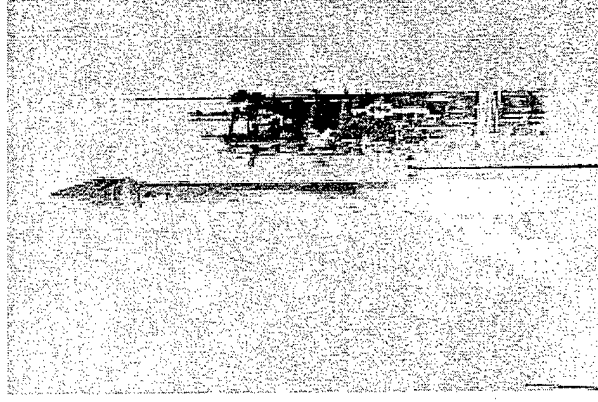
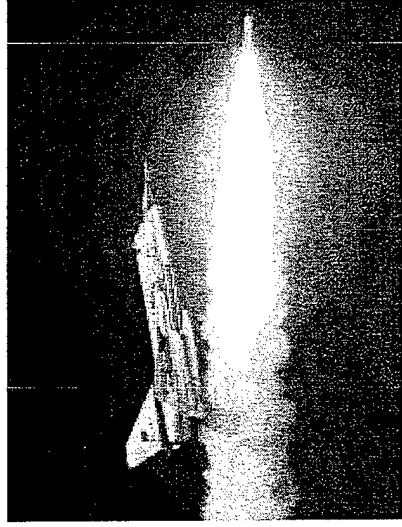
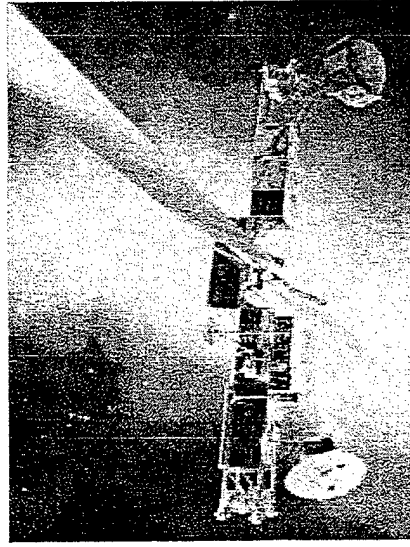
High Energy Density Materials (HEDM) Program Objective



*Breaking the
performance barrier*

Identify and develop advanced chemical propellants for rocket propulsion applications

- Hydrocarbons for liquid boosters
- Liquid & solid oxidizers for boost and upper stages
- Monopropellants for upper stages and satellites
- Cryogenic propellants for upper stages





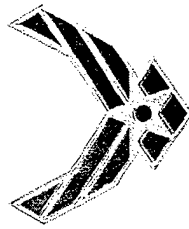
HEDM Propellant Payoffs

"The highest leverage technology area impacting launch vehicles is the development of high-energy-density materials for use as propellants."

-- New World Vistas Panel on Space Technology (1995)

Vehicle Type	Baseline Vehicle	Propellant	Takeoff Mass (lb)	Payload Mass (lb)	Payload Mass (lb) With 10% Isp Increase
Two-stage ELV	Atlas II // Centaur D-1A	RP-1/LOX (Isp = 295 s) // LH2/LOX (Isp = 455 s)	360,000	12,500	15,600 (+25%)
SSTO RLV	Lockheed SSTO	LH2/LOX (Isp = 455 s)	1,900,000	40,000	68,000 (+70%)
Missile Defense Interceptor	Boost-Phase Interceptor	HTPB/Al/HMX (Isp = 270 s)	1,847	74	110 (+49%)

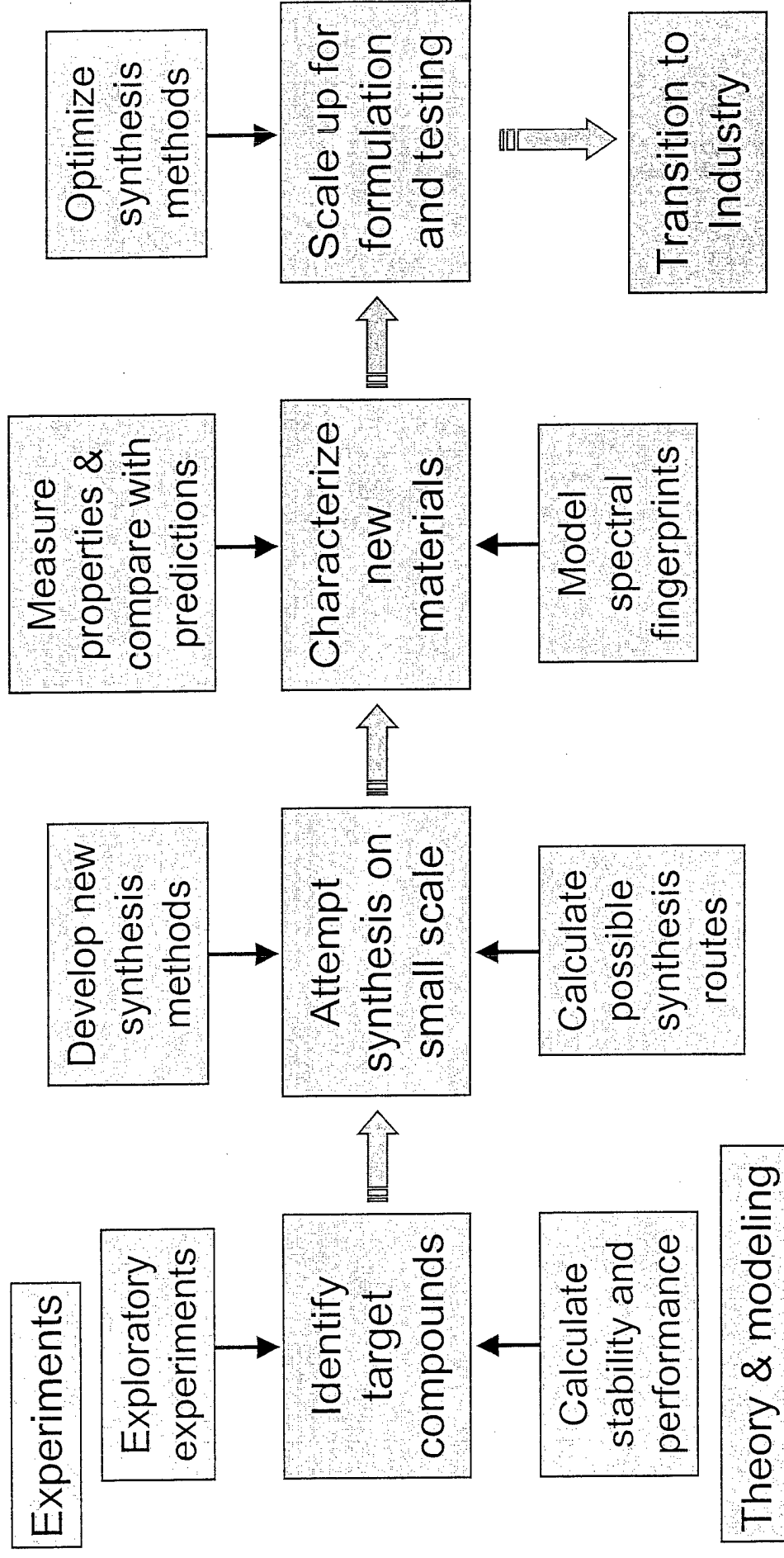
Our research is aimed at increasing propellant Isp by 5 to 50%

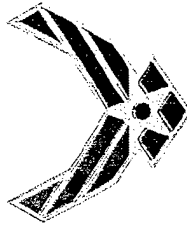


HEDM Program General Approach



Employ a synergic blend of experimental, theoretical, and computational techniques derived from the disciplines of chemistry and physics





The Calculation of Molecular Properties



04

Various computational techniques are employed to solve the molecular electronic Schrödinger equation from quantum mechanics:

$$\left[-\frac{1}{2} \sum_i \nabla_i^2 - \sum_i \sum_{\alpha} \frac{Z_{\alpha}}{r_{i\alpha}} + \sum_i \sum_{j>i} \frac{1}{r_{ij}} \right] \Psi_{el} = E_{el} \Psi_{el}$$

Determining what to synthesize:

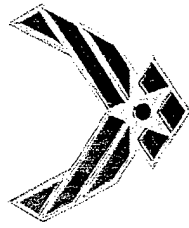
Thermodynamic properties relate directly to propellant performance and are obtained from relative energies of reactants, intermediates, and products

Determining how to synthesize them:

Potential-energy surfaces – energy profiles associated with all degrees of freedom in a chemical system – give insight into stabilities and reaction & decomposition pathways

Determining whether we've made what we wanted to make:

Structures and spectra (IR, Raman, NMR) are obtained by evaluating derivatives of the energy or other properties with respect to nuclear coordinates or applied fields



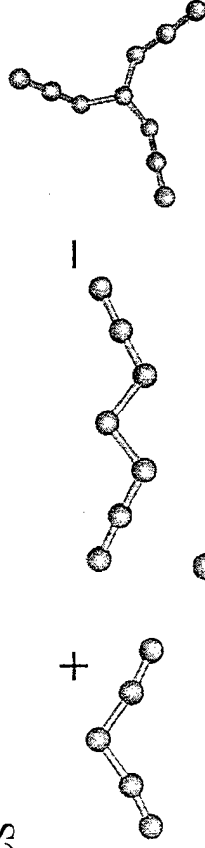
DARPA Polynitrogen Program



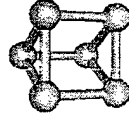
Program began late FY98

Six groups funded to discover, scale up, and demonstrate polynitrogen propellants or explosives

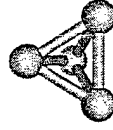
AFRL / Edwards



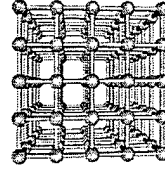
Naval Research Laboratory



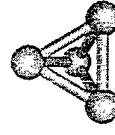
Los Alamos National Laboratory



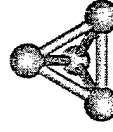
Lawrence Livermore National Laboratory



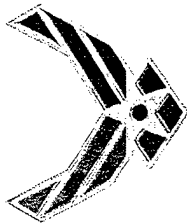
Colorado School of Mines / National Renewable Energy Laboratory



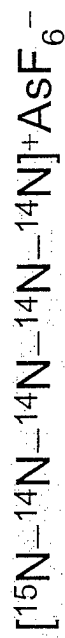
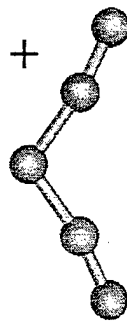
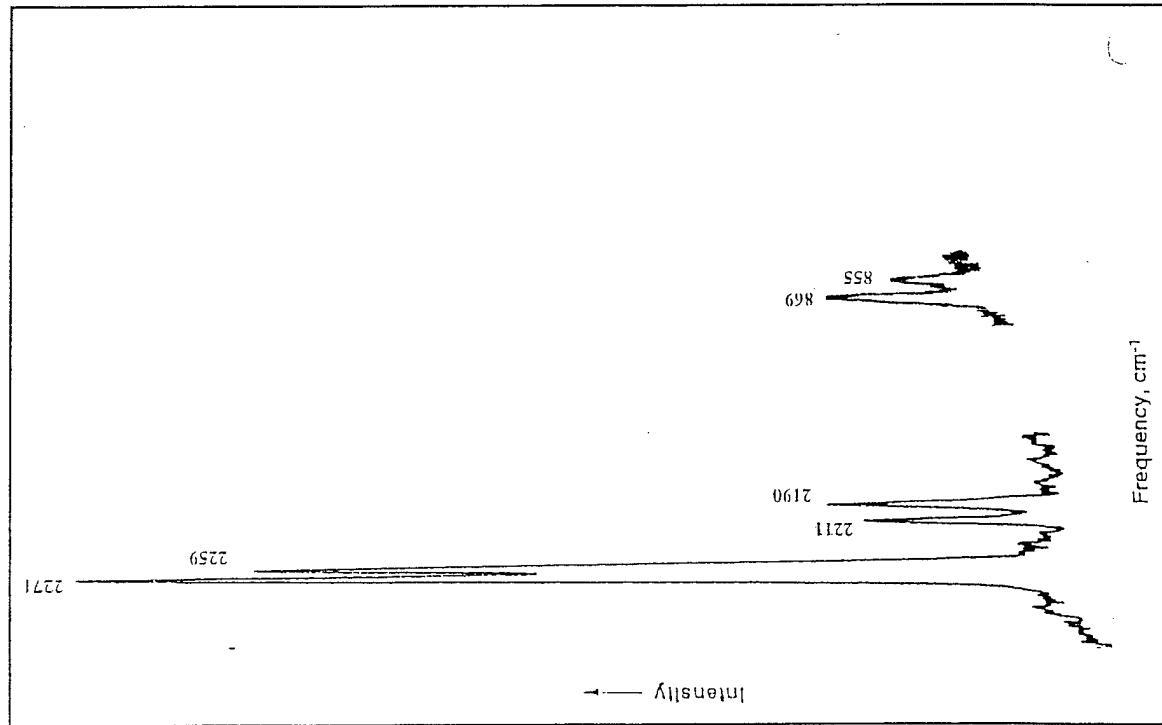
Defense Research Establishment, Sweden



Only the AFRL group has been successful



Identifying a Completely New Molecule: Comparison of Calculated and Measured Spectra



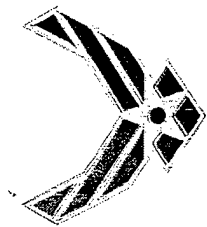
and



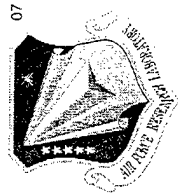
$^{14}\text{N} - ^{15}\text{N}$ Isotopic Shifts (cm^{-1})

Mode	Obs.	Calc. [†]
$\nu_1(a_1)$	12	11.8
$\nu_7(b_2)$	21	21.4
$\nu_2(a_1)$	14	14.1

[†]CCSD(T)/6-311+G(2d) results

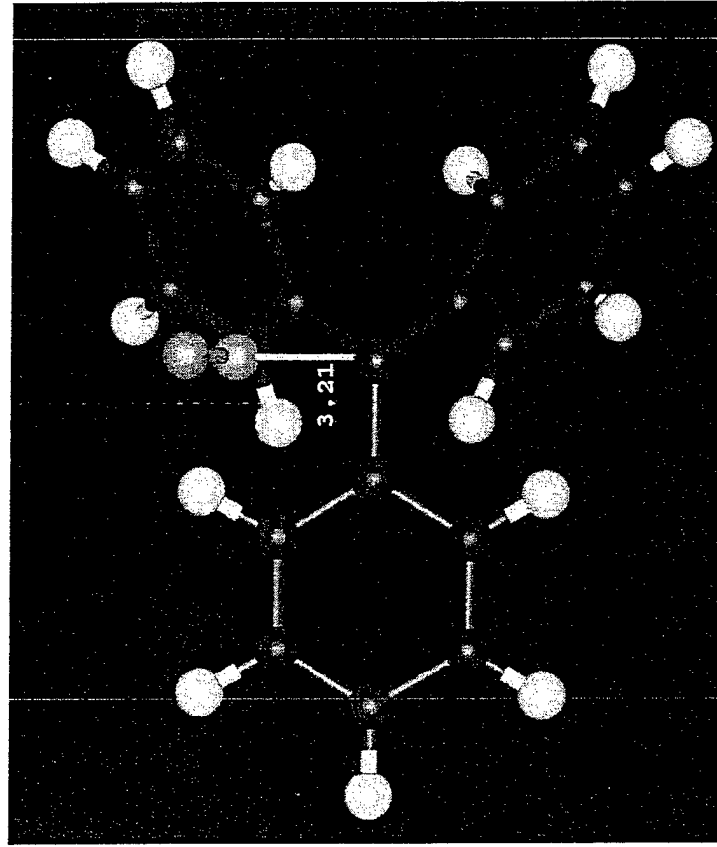
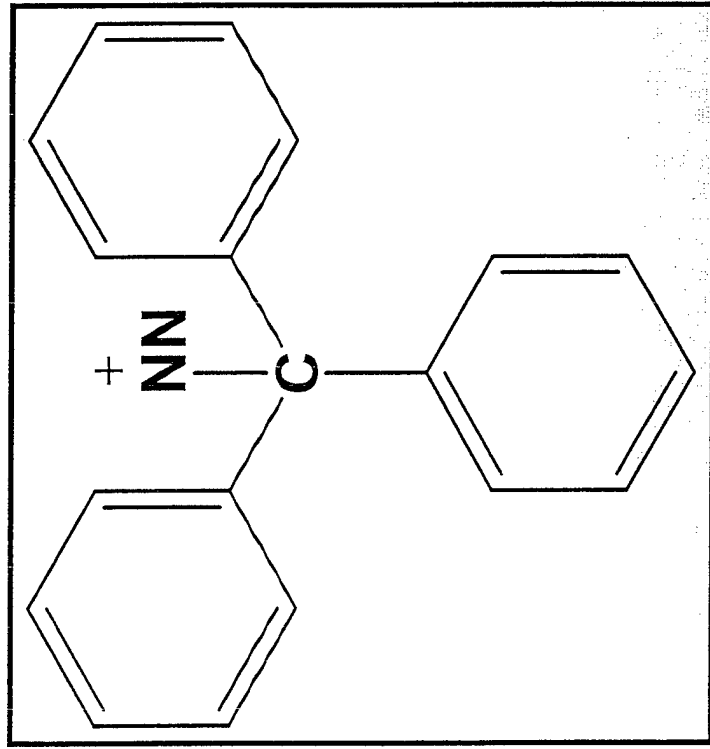


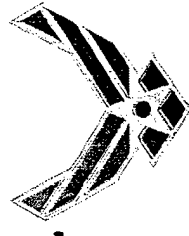
Identifying Potential Polynitrogen Precursors



*This ion has been suggested
as a useful precursor to new
polynitrogen molecules...*

*... but calculations predict it to be
unstable.*





Summary

Computational chemistry plays a critical role in HEDM research

Guides the choice of target compounds and possible synthetic routes, provides verification of successful synthesis.

CC is addressing an ever wider range of Air Force applications

New methods are under development (e.g., modeling chemistry in solution or on surfaces). Parallel computing technology has greatly expanded the scope of problems which can be modeled.

Access to high performance computing resources is essential

Many quantum chemical calculations are too costly and complex to perform on "standard" platforms (e.g., standalone workstations or desktop Linux PCs).